CHBE 305

COMPUTATIONAL METHODS IN CHEMICAL ENGINEERING

Spring 2020

Instructor

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Office Hours: MW 4 - 5 PM (or by appointment)

Course Contents

1. **Introduction**: Approximations and round-off errors; truncation errors; Taylor series.
2. **Systems of linear algebraic equations**: Introduction; Gauss elimination, LU decomposition; inversion of matrices; error analysis and system condition; solution of boundary value problems with finite differences; triangular and band matrices; Iterative methods; Gauss-Seidel method.
3. **Curve fitting**: Least squares regression; linear regression; polynomial regression; multiple linear regression; general linear least squares; nonlinear regression. Interpolation; spline interpolation.
4. **Non-linear equations**: Bisection method; false-position method; simple fixed-point iteration; Newton-Raphson method; secant method; multiple roots; systems of nonlinear equations; roots of polynomials.
5. **Numerical integration**: Trapezoidal and Simpson's rules; Romberg integration; Gauss quadrature.
6. **Ordinary differential equations**: Euler's methods; Runge-Kutta methods; adaptive Runge-Kutta methods; systems of equations; stiffness; multistep methods; general methods for boundary value problems.

ABET Outcomes

The ABET student outcome that will be evaluated in this course is:

SO 3: An ability to communicate effectively with a range of audiences.

Textbook

S. C. Chapra and R.R. Canale, "Numerical methods for Engineers." 7th Edition, McGraw-Hill (2015).

Recitation Sessions (Computer Labs)

A 2-hour recitation session will be held every week. Attendance of recitation sessions is mandatory.

Homework Assignments

Six to eight homework problem sets will be assigned during the semester. Problems will involve both theoretical analysis and computer programing. Students should use MATLAB for the solution of homework problems.

Homework Policy

- Late homework will be penalized, unless prior permission has been obtained from the instructor.
- Homework that is more than two days late will not be accepted.
- The submission and grading procedures are described in detail in a separate document posted on Canvas in the folder “Syllabus, Schedule and Policies.”

Test and Quizzes

There will be three (3) short quizzes after the completion of major topics to test the students' understanding of key concepts. The quizzes will not require programming or the use of computers and their dates are listed on the course schedule.

There will also be a comprehensive test on March 25 on all the material covered during the two thirds of the semester. Again, the test will focus on concepts and will not require programming or the use of computers.

Team Project

Students will work in teams to design a chemical reactor system that meets certain specifications. Each team will:

- prepare a 2-page preliminary written report (due on March 13, 2020),
- make a formal presentation of their design (scheduled during finals week), and
- submit a final written report by the last day of finals (May 6, 2020).

Between March 23 and March 27, students will work with CAPC coaches who will review their 2-page written report on the project and provide feedback (not grades) to help the teams improve their writing. A revised version of this assignment will be due on March 30. Both the preliminary and the final versions of the report will be graded.

During the last two weeks of classes, the teams will work again with CAPC coaches to prepare their final project presentations. The presentations will be scheduled during the week of finals.

Professional Communications

The professional communication component of this course will include two lectures presented by team members from Rice's Center for Academic and Professional Communication (CAPC):

- A lecture on creating effective graphics (tentatively scheduled for February 3)
- A lecture on designing effective presentations (tentatively scheduled for March 23)

Grading Policy

- Homework: 30%
- Quizzes: 20% (10% for each of the best 2 out of 3)
- Comprehensive test: 20%
- Project: 30%

Note that the weights of the course components may change.

Honor Code Policy

“You may talk to other students in your CHBE 305 class, the course TAs, and the instructor about any course assignment that is not specifically designated as pledged. The assistance you may receive from other students in your CHBE 305 class should be strictly limited to a discussion about the fundamental concepts involved in solving the problem(s). You are not allowed to share calculation details and computer codes, or to consult another student's solution (even from a previous CHBE 305 or another numerical methods class). Submitted solutions to assignments may not be copied from any source.”

ADA Statement

Any student with a documented disability needing academic adjustments or accommodations is requested to speak with the instructor during the first two weeks of class. All discussions will remain confidential. Students with disabilities will need to also contact Disability Support Services in the Ley Student Center.